Amendments to the Claims:

Please cancel claims 1-18 without disclaimer or prejudice to applicants' right to purse the subject matter of these claims in a future continuation or divisional application.

Please add new claims 19-34 as set forth below.

1-18. (Canceled)

19. (New) A method for determining a free energy of binding of a potential inhibitor to an enzyme, comprising the steps of:

obtaining a structure and a free energy of binding to said enzyme for each of two or more enzyme substrates or inhibitors;

orienting said structures of said two or more enzyme substrates or inhibitors for maximum geometric coincidence with each other;

determining an electrostatic potential at each of more than one point on a van der Waals surface of each of said enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of each of said enzyme substrates or inhibitors onto a geometric surface of one of said two or more enzyme substrates or inhibitors, each of said two or more enzyme substrates or inhibitors being thereby described by an identical surface geometry but a different electrostatic potential surface, and each of said electrostatic potentials being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials, said positional information, and said known free energy of binding of one of said two or more enzyme substrates or inhibitors into a neural network;

thereafter, training said neural network until said neural network predicts said free energy of binding of said one of said two or more enzyme substrates or inhibitors;

repeating said steps of inputting and training for each of the remaining said two or more enzyme substrates or inhibitors to produce a trained network;

thereafter, determining a potential inhibitor electrostatic potential at each of more than one point on a van der Waals surface of said potential inhibitor, said potential inhibitor having a known structure and an unknown free energy of binding to said enzyme;

orienting said structure of said potential inhibitor for maximum geometric coincidence with said structures of said two or more enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of said potential inhibitor onto a geometric surface of one of said two or more enzyme substrates or inhibitors, said potential inhibitor having a surface geometry identical to that of said two or more enzyme substrates or inhibitors, but a different electrostatic potential surface, and each of said electrostatic potentials of said potential inhibitor being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials and said positional information of said electrostatic potentials of said potential inhibitor into said trained network; and

using said trained network to calculate a free energy of binding of said potential inhibitor to said enzyme.

20. (New) A computer readable medium, comprising:

computer-readable information;

said information capable of interacting with a computer to produce an output;

said output being a calculated free energy of binding of a potential inhibitor to an enzyme;

said output being calculated by:

orienting structures of two or more enzyme substrates or inhibitors for maximum geometric coincidence with each other;

each of said two or more enzyme substrates or inhibitors having a predetermined structure and a predetermined free energy of binding to said enzyme;

determining an electrostatic potential at each of more than one point on a van der Waals surface of each of said enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of each of said enzyme substrates or inhibitors onto a geometric surface of one of said two or more enzyme substrates or inhibitors, each of said two or more enzyme substrates or inhibitors being thereby described by an identical surface geometry but a different electrostatic potential surface, and each of said electrostatic potentials being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials, said positional information, and said known free energy of binding of one of said two or more enzyme substrates or inhibitors into a neural network;

thereafter, training said neural network until said neural network predicts said free energy of binding of said one of said two or more enzyme substrates or inhibitors;

repeating said steps of inputting and training for each of the remaining said two or more enzyme substrates or inhibitors to produce a trained network;

thereafter, determining a potential inhibitor electrostatic potential at each of more than one point on a van der Waals surface of said potential inhibitor, said potential inhibitor having a known structure and an unknown free energy of binding to said enzyme;

orienting said structure of said potential inhibitor for maximum geometric coincidence with said structures of said two or more enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of said potential inhibitor onto a geometric surface of one of said two or more enzyme substrates or inhibitors, said potential inhibitor having a surface geometry identical to that of said two or more enzyme substrates or inhibitors, but a different electrostatic potential surface, and each of said electrostatic potentials of said potential inhibitor being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials and said positional information of said electrostatic potentials of said potential inhibitor into said trained network; and

using said trained network to calculate a free energy of binding of said potential substrate to said enzyme.

21. (New) A method for determining a free energy of binding of a potential substrate to an enzyme, comprising the steps of:

obtaining a structure and a free energy of binding to said enzyme for each of two or more enzyme substrates or inhibitors;

orienting said structures of said two or more enzyme substrates or inhibitors for maximum geometric coincidence with each other;

determining an electrostatic potential at each of more than one point on a van der Waals surface of each of said enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of each of said enzyme substrates or inhibitors onto a geometric surface of one of said two or more enzyme substrates or inhibitors, each of said two or more enzyme substrates or inhibitors being thereby described by an identical surface geometry but a different electrostatic potential surface, and each of said electrostatic potentials being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials, said positional information, and said known free energy of binding of one of said two or more enzyme substrates or inhibitors into a neural network;

thereafter, training said neural network until said neural network predicts said free energy of binding of said one of said two or more enzyme substrates or inhibitors;

repeating said steps of inputting and training for each of the remaining said two or more enzyme substrates or inhibitors to produce a trained network;

thereafter, determining a potential substrate electrostatic potential at each of more than one point on a van der Waals surface of said potential substrate, said

potential substrate having a known structure and an unknown free energy of binding to said enzyme;

orienting said structure of said potential substrate for maximum geometric coincidence with said structures of said two or more enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of said potential substrate onto a geometric surface of one of said two or more enzyme substrates or inhibitors, said potential substrate having a surface geometry identical to that of said two or more enzyme substrates or inhibitors, but a different electrostatic potential surface, and each of said electrostatic potentials of said potential substrate being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials and said positional information of said electrostatic potentials of said potential substrate into said trained network; and

using said trained network to calculate a free energy of binding of said potential substrate to said enzyme.

22. (New) A computer readable medium, comprising:

computer-readable information;

said information capable of interacting with a computer to produce an output;

said output being a calculated free energy of binding of a potential substrate to an enzyme;

said output being calculated by:

orienting structures of two or more enzyme substrates or inhibitors for maximum geometric coincidence with each other;

each of said two or more enzyme substrates or inhibitors having a predetermined structure and a predetermined free energy of binding to said enzyme;

determining an electrostatic potential at each of more than one point on a van der Waals surface of each of said enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of each of said enzyme substrates or inhibitors onto a geometric surface of one of said two or more enzyme substrates or inhibitors, each of said two or more enzyme substrates or inhibitors being thereby described by an identical surface geometry but a different electrostatic potential surface, and each of said electrostatic potentials being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials, said positional information, and said known free energy of binding of one of said two or more enzyme substrates or inhibitors into a neural network;

thereafter, training said neural network until said neural network predicts said free energy of binding of said one of said two or more enzyme substrates or inhibitors;

repeating said steps of inputting and training for each of the remaining said two or more enzyme substrates or inhibitors to produce a trained network;

thereafter, determining a potential substrate electrostatic potential at each of more than one point on a van der Waals surface of said potential

substrate, said potential substrate having a known structure and an unknown free energy of binding to said enzyme;

orienting said structure of said potential substrate for maximum geometric coincidence with said structures of said two or more enzyme substrates or inhibitors;

thereafter, mapping each of said electrostatic potentials of said potential substrate onto a geometric surface of one of said two or more enzyme substrates or inhibitors, said potential substrate having a surface geometry identical to that of said two or more enzyme substrates or inhibitors, but a different electrostatic potential surface, and each of said electrostatic potentials of said potential substrate being described by positional information relating said electrostatic potentials to said geometric surface;

thereafter, inputting said electrostatic potentials and said positional information of said electrostatic potentials of said potential substrate into said trained network; and

using said trained network to calculate a free energy of binding of said potential substrate to said enzyme.

23. (New) The method of claim 19, wherein the neural network contains an input layer, a hidden layer, and an output layer, and is a feed forward network with back propagation of error that learns with momentum.

24. (New) The method of claim 23, wherein the network uses between 4 and 12 hidden layer neurons, a learning rate between 0.1 and 0.5, a momentum term between 0.8 and 0.9, and between 5×10^3 and 1×10^6 learning iterations.

25. (New) The method of claim 24, wherein the number of hidden layer neurons, number of iterations, learning rate, and momentum can be adjusted so that the network outputs a binding energy with 98% accuracy.

26. (New) The computer readable medium of claim 20, wherein the neural network contains an input layer, a hidden layer, and an output layer, and is a feed forward network with back propagation of error that learns with momentum.

27. (New) The computer readable medium of claim 26, wherein the network uses between 4 and 12 hidden layer neurons, a learning rate between 0.1 and 0.5, a momentum term between 0.8 and 0.9, and between 5×10^3 and 1×10^6 learning iterations.

28. (New) The computer readable medium of claim 27, wherein the number of hidden layer neurons, number of iterations, learning rate, and momentum can be adjusted so that the network outputs a binding energy with 98% accuracy.

29. (New) The method of claim 21, wherein the neural network contains an input layer, a hidden layer, and an output layer, and is a feed forward network with back propagation of error that learns with momentum.

30. (New) The method of claim 29, wherein the network uses between 4 and 12 hidden layer neurons, a learning rate between 0.1 and 0.5, a momentum term between 0.8 and 0.9, and between 5×10^3 and 1×10^6 learning iterations.

31. (New) The method of claim 30, wherein the number of hidden layer neurons, number of iterations, learning rate, and momentum can be adjusted so that the network outputs a binding energy with 98% accuracy.

32. (New) The computer readable medium of claim 22, wherein the neural network contains an input layer, a hidden layer, and an output layer, and is a feed forward network with back propagation of error that learns with momentum.

33. (New) The computer readable medium of claim 32, wherein the network uses between 4 and 12 hidden layer neurons, a learning rate between 0.1 and 0.5, a momentum term between 0.8 and 0.9, and between 5×10^3 and 1×10^6 learning iterations.

34. (New) The computer readable medium of claim 33, wherein the number of hidden layer neurons, number of iterations, learning rate, and momentum can be adjusted so that the network outputs a binding energy with 98% accuracy.